2-Pentyl-oxirane-2-carboxylic acid methyl ester

Inchi: InChI=1S/C9H16O3/c1-3-4-5-6-9(7-12-9)8(10)11-2/h3-7H2,1-2H3
InchiKey: RXFVDNPJQQLKTM-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: CCCCCC1(C(=O)OC)CO1
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
gf	-239.88	kJ/mol	Joback Method
hf	-517.85	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.509		Crippen Method
mcvol	140.120	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1192.00		NIST Webbook
rinpol	1192.00		NIST Webbook
tb	515.54	K	Joback Method
tc	709.26	K	Joback Method
tf	331.76	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.06	J/mol×K	515.54	Joback Method
cpg	352.66	J/mol×K	547.83	Joback Method
cpg	365.46	J/mol×K	580.11	Joback Method
cpg	377.54	J/mol×K	612.40	Joback Method
cpg	389.00	J/mol×K	644.69	Joback Method
cpg	399.91	J/mol×K	676.98	Joback Method
cpg	410.35	J/mol×K	709.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume